

Metal-insulator transition in an one-dimensional half-filled interacting mesoscopic ring with spinless fermions: Exact results

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We calculate persistent current of one-dimensional rings of fermions neglecting the spin degrees of freedom considering only nearest-neighbor Coulomb interactions with different electron fillings in both ordered and disordered cases. We treat the interaction exactly and find eigenenergies by exact diagonalization of many-body Hamiltonian and compute persistent current by numerical derivative method. We also determine Drude weight to estimate the conducting nature of the system. From our numerical results, we obtain a metal-insulator transition in half-filled case with increasing correlation strength U but away from half-filling no such transition is observed even for large U .

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I. INTRODUCTION

The metal-insulator (MI) transition is one of the most significant phenomena in condensed matter physics^{1–5}. The usual band structure predictions are not capable of exploring many experimental evidences. For example, according to the band structure analysis, Iron(II) Oxide (FeO), Nickel Oxide (NiO) and Cobalt Oxide (CoO) are shown to be metallic but experimentally they exhibit insulating phase. Similarly, the absence of magnetism in several high-temperature superconductors verified in experiments contradict theoretical results which suggest finite magnetism. Likewise a strong mismatch has also been observed between theoretical predictions and experimental observation in the determination of band-gap for many semi-conductors⁴. Considering Hubbard correlation, when people calculate the electronic band structures, it has flourished all the experimental results quiet strongly. If the Hubbard correlation is much greater than the bandwidth of a material, the MI transition becomes extremely relevant, and, compounds containing rare earth ions with localized $4f$ electrons or partially filled d -band elements show this type of transition. On the other hand, if bandwidth is higher than the Hubbard correlation, then the electron-electron interaction can be excluded and the experimental evidences for those systems can be explained by conventional band structure predictions⁴. It is not only true for the macroscopic bulk systems but Hubbard correlation has an effective impact on low-dimensional transport phenomena^{6,7}.

Persistent current in an isolated 1D small conducting ring threaded by a magnetic flux is a well established phenomenon in mesoscopic regime. There exist many controversial issues involving current amplitude, sign and its periodicity between theoretical and experimental results^{6–21}, and in last few decades people have attempted a lot to remove these discrepancies by improving their models^{6,7,19–21}. But still, it is an open challenge to remove the disparity exactly. People have also explored the role of interactions on persistent current and to some extent the enhancement of current has been observed in presence of

interaction⁷. In the early 90's Bouzerar *et al.* have performed the calculation of persistent current in 1D ring considering spinless electrons. Utilizing a Wigner-Jordan transformation on the tight-binding (TB) Hamiltonian they have found the ground state energy from Lanczos algorithm and determined the current using conventional method. It has been shown that the ring exhibits a MI transition at the half-filled band case due to correlation, and, away from half-filling the interaction has no such strong influence⁶. Studying persistent current in finite

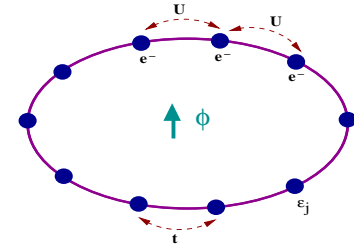


FIG. 1: (Color online). 1D ring with interacting spinless electrons threaded by an AB flux ϕ where the filled blue circles represent the atomic sites.

two-dimensional (2D) arrays of semiconducting quantum dots in presence of magnetic field perpendicular to the 2D plane the phenomenon of MI transition in the half-filled band case has also been reported in a nice work²² by Das Sarma and his co-worker. However, the persistent current in 2D quantum dot arrays has important differences compared to established persistent current in one-dimensional ring structure subjected to Aharonov-Bohm (AB) flux ϕ . In that work (Ref.²²) several qualitative features of persistent current as functions of both on-site and extended electron-electron interactions have been put forward where the current has been computed by determining ground state energy through Lanczos diagonalization technique. Here it is important to note that the understanding of the MI transition in 1D system of spinless fermions in other context has already been established several years ago where response functions have been calculated²³ in a solvable model. These response

functions, on the other hand, cannot be computed by Bethe ansatz though this ansatz allows us to get rigorous statements on many-body system of interacting 1D spinless fermions^{24–26}.

The aim of this paper is to treat the interacting Hamiltonian *exactly* and find ground state energy from exact diagonalization of many-body TB Hamiltonian. Evaluating ground state energy we compute persistent current using conventional method both for ordered and disordered cases. Our model comprises a 1D finite ring of spinless fermions with nearest-neighbor (NN) Coulomb correlation. From our analysis we find that in the limit of half-filling current amplitude decreases sharply with correlation strength U and drops to almost zero (insulating phase) for moderate U , while a metallic phase is always observed in the non-half-filled cases irrespective of U . To substantiate the role of U more precisely on conducting properties, in the present work, we also discuss the variation of Drude weight²⁷ for different electron fillings, and, from these results sharp transition between two conducting phases is noticed. Finally, we discuss scaling behavior of persistent current with ring size.

The rest of the work is arranged as follows. Section II describes the model and theoretical approach and Sec. III presents the numerical results. Finally, we summarize our findings in Sec. IV.

II. MODEL AND FORMALISM

The model is shown in Fig. 1 where we consider an AB ring of spinless fermions with nearest-neighbor Coulomb interaction. Under nearest-neighbor hopping approximation the TB Hamiltonian of such a N -site ring reads,

$$\mathbf{H} = \sum_j \epsilon_j n_j - t \sum_j \left[e^{i\theta} c_j^\dagger c_{j+1} + e^{-i\theta} c_{j+1}^\dagger c_j \right] + U \sum_{j=1} n_j n_{j+1} \quad (1)$$

where c_j^\dagger and c_j are the usual creation and annihilation operators, respectively, ϵ_j describes the site energy, t is the NN hopping integral and U measures the NN Coulomb interaction. The phase factor $\theta (= 2\pi\phi/N\phi_0)$ arises due to AB flux ϕ , where $\phi_0 = ch/e$. For ordered ring, all site energies are identical and therefore we set them to zero without loss of generality. While, for disordered rings we choose site energies randomly from a ‘Box’ distribution function of width W within the range $-W/2$ and $W/2$.

To find ground state energy of the system first we construct the many-body Hamiltonian matrix considering the interaction exactly where the matrix elements are obtained following the prescription: $\mathbf{H}_{mn} = \langle \psi_m | \mathbf{H} | \psi_n \rangle$. Here $|\psi_m\rangle$ and $|\psi_n\rangle$ are the basis vectors associated with total number of spinless fermions N_e in the ring. For example, for a two-electron system we define them as $|\psi_m\rangle = c_p^\dagger c_q^\dagger |0\rangle$ and $|\psi_n\rangle = c_k^\dagger c_l^\dagger |0\rangle$ where $|0\rangle$ is the null

state. Likewise we define basis vectors for higher-electron systems and construct appropriate matrices. Once the matrix is constructed, we compute ground state energy by exact diagonalization method.

The persistent current in such a system at absolute zero temperature ($T = 0$ K) can be determined from the relation¹⁷, $I(\phi) = -\partial E_0(\phi)/\partial\phi$, where $E_0(\phi)$ is the ground state energy.

Finally, we calculate Drude weight D from the expression²⁷,

$$D = \frac{N}{4\pi^2} \left[\frac{\partial^2 E_0(\phi)}{\partial\phi^2} \right]_{\phi \rightarrow 0}. \quad (2)$$

Finite value of D corresponds to the metallic phase while it drops to zero for the insulating one, as originally put forward by Kohn.

III. RESULTS AND DISCUSSIONS

Below we present our results. In our numerical calculations we choose $c = e = \hbar = 1$ and measure the energy in unit of t which is fixed at 1 eV. Since we are dealing with exact many-body Hamiltonian, dimension of the matrix increases sharply with electron filling, and therefore, we restrict ourselves to the rings with few electrons due to computation limitations. But, the point is that with these results we can easily analyze the characteristic features of current as well as conducting properties for larger rings with higher N_e as all the basic features will remain invariant with our numerical results presented here.

Figure 2 displays the current-flux characteristics of some typical ordered half-filled mesoscopic rings for three

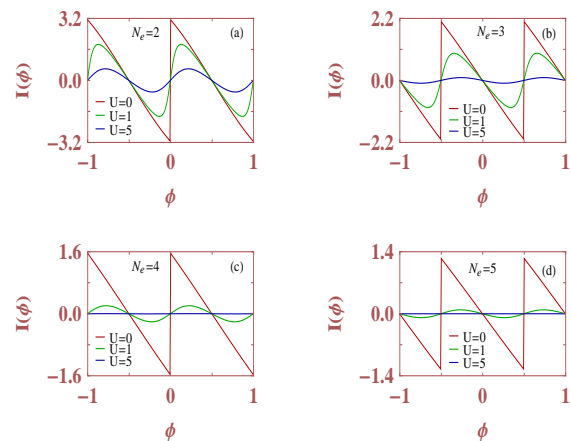


FIG. 2: (Color online). $I(\phi)$ vs ϕ characteristics for three distinct values of U in the ordered ($W = 0$) half-filled ($N_e = N/2$) rings where (a), (b), (c) and (d) correspond to $N = 4, 6, 8$ and 10 , respectively.

distinct values of correlation strength U where (a), (b), (c) and (d) correspond to $N = 4, 6, 8$ and 10 , respectively. In the absence of Coulomb correlation, current

exhibits sharp transitions at $\phi = 0$ (for even N_e) or ± 0.5 (for odd N_e) associated with the energy level crossing, while it becomes continuous as long as interaction is included. Most interestingly we see that for a specific U current decreases sharply as we increase ring size, and, for large U it practically drops to zero (blue line). This

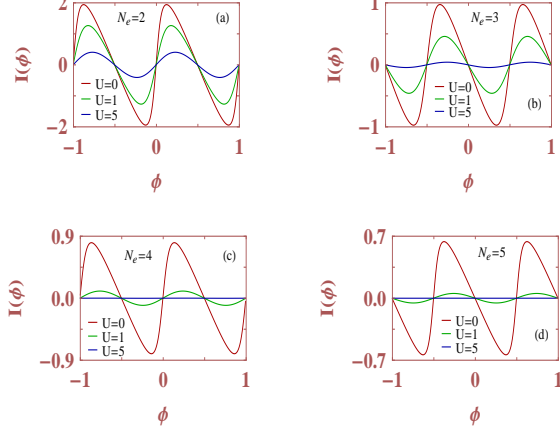


FIG. 3: (Color online). Current-flux characteristics in disordered ($W = 2$) half-filled rings for the identical parameter values taken in Fig. 2.

is solely due to the repulsive Coulomb interaction U . In the limit of half-filling all sites are occupied by single electrons and their hopping to the neighboring sites strongly depend on the two physical parameters, viz, t and U . For

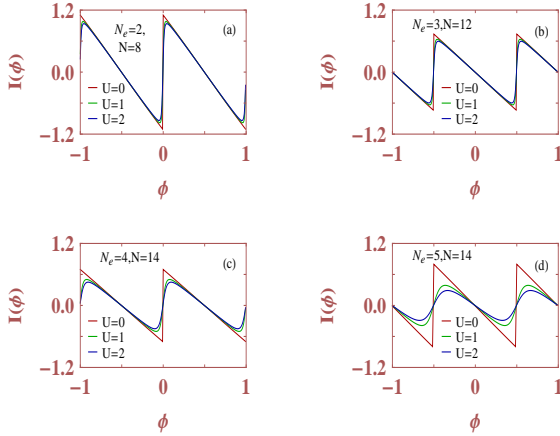


FIG. 4: (Color online). $I(\phi)$ vs ϕ characteristics for three different values of U in some ordered non-half-filled rings.

low U , when NN hopping dominates finite current is obtained, exhibiting a *conducting phase*. While for large U , the repulsive interaction gets significant which suppresses electron hopping from one site to the neighboring sites and it becomes more effective for larger ring. Therefore, current gets decreased with U and with increasing ring size it almost vanishes to zero which yields the *insulating phase*.

Certainly, further reduction of current is obtained when we include the effect of disorder in such half-filled interacting rings as disorder itself tries to localize the energy levels. The results of some typical disordered rings

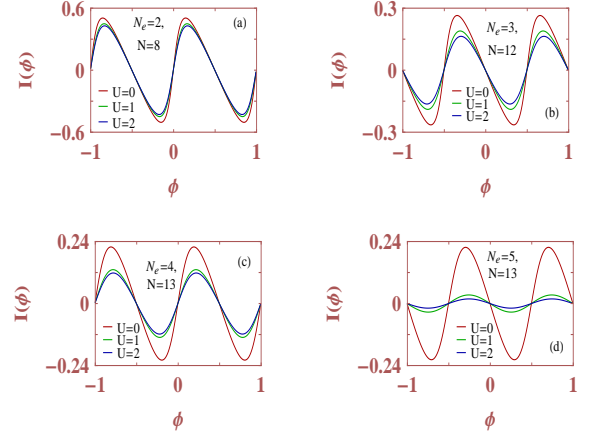


FIG. 5: (Color online). $I(\phi)$ - ϕ characteristics for different values of U in some typical disordered ($W = 2$) non-half-filled rings.

are shown in Fig. 3, where the averaging over fifty distinct disordered configurations are taken into account. Clearly we see that a significant reduction of current takes place solely due to W , providing a continuous variation with ϕ because of the complete removal of degenerate energy

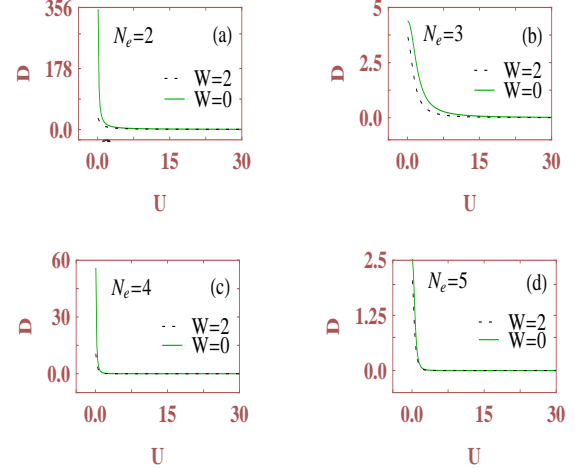


FIG. 6: (Color online). Variation of Drude weight D (in unit of $N/4\pi^2$) as a function of U in the half-filled limit for both the ordered and disordered rings.

levels, and it is further suppressed by the repulsive factor U .

The situation becomes completely different when the rings are less than half-filled. To reveal this fact in Fig. 4 we show the current-flux characteristics of some typical ordered mesoscopic rings where we set $N_e < N/2$. For these non-half-filled rings the rate of decrease of current

with U is too small and cannot be absolute zero even for a very large U . The reason is that for such rings empty sites are always available where electrons can hop from the filled sites to these empty sites providing a net

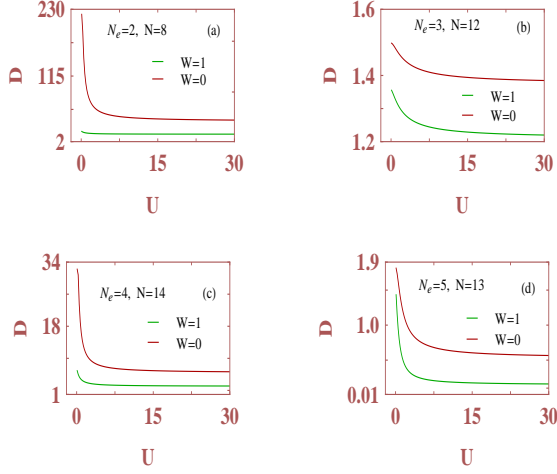


FIG. 7: (Color online). D (in unit of $N/4\pi^2$) vs U in the non-half-filled rings for both ordered and disordered cases.

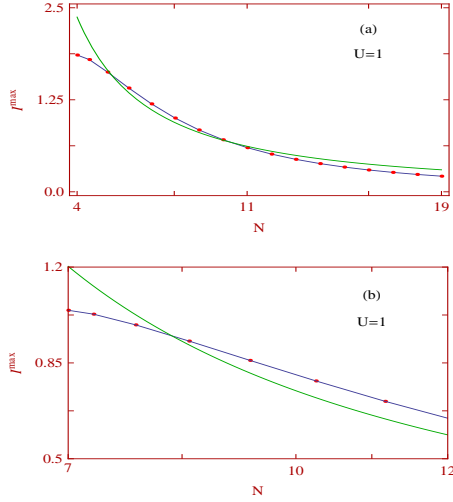


FIG. 8: (Color online). Variation of persistent current with ring size N considering $U = 1$ and $W = 0$. The red dots, corresponding to the currents, are evaluated from our presented scheme and joining these dots a continuous blue line is obtained. Using these dots we find a scaling relation between the current and ring size which generates the green line. Two cases are analyzed depending on N_e where (a) and (b) correspond to $N_e = 2$ and 3 , respectively.

circular current. Thus the rings exhibit only conducting phase and insulating phase is no longer available when $N_e < N/2$, even for very large U .

Almost identical picture is also obtained even if we consider the effect of disorder in these non-half-filled interacting rings. Though current gets reduced with W

itself, the existence of empty sites always provides a net current as clearly seen from the spectra given in Fig. 5.

The interplay between electron filling and Coulomb correlation on electronic motion can be much more clearly explained by measuring Drude weight D , which essentially determines conducting nature of the system. In Fig. 6 we show the variation of Drude weight D as a function of U for some typical half-filled rings for both the ordered and disordered cases. Interestingly we see that for all these rings Drude weight falls sharply to zero even for a slight increment of U which reveals a crossover from the conducting to the insulating phase of the system.

This insulating phase is no longer available even when the repulsive interaction is too high for less than half-filled rings. This behavior is presented in Fig. 7 where we plot the D - U characteristics for both the ordered and

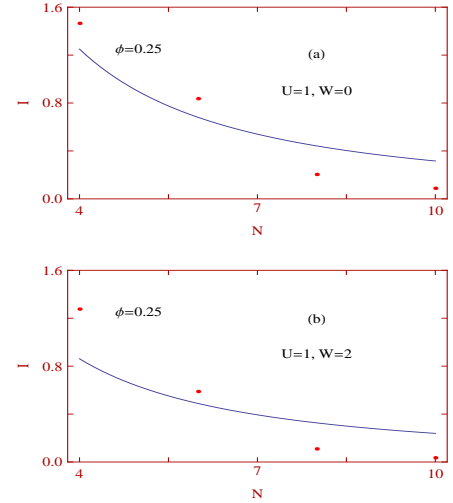


FIG. 9: (Color online). Dependence of persistent current with ring size N in the half-filled band case when the Coulomb correlation strength is fixed at $U = 1$. The red dots, corresponding to the currents, are evaluated from our presented scheme and using these dots we find a scaling relation between I and N which produces the green line. Two cases are analyzed depending on disorder strength W where (a) and (b) correspond to $W = 0$ and 2 , respectively.

disordered rings, like above in Fig. 6, when $N_e < N/2$. Though in presence of disorder electrical conductivity, viz, D decreases but it never drops to zero, providing the metallic nature of the system.

To make the present communication a self contained study now we focus our attention on the variation of persistent current with ring size N and from it we try to figure out the scaling behavior.

In Fig. 8 we present the variation of I^{\max} with system size N taking the maximum absolute value of persistent current from the current-flux curve (considering the variation of ϕ from 0 to ϕ_0). Two cases are analyzed depending on N_e , where (a) and (b) correspond to $N_e = 2$ and 3 , respectively, and in both these cases we set $U = 1$. The red dots, representing the currents,

are determined from our presented scheme (described in Sec. II) and connecting these dots we get the continuous blue lines. With this dots we establish a scaling relation of the form: $I^{\max} = CN^{-\xi}$ where the exponent ξ becomes 1.33 both for $N_e = 2$ and 3 which we find from our extensive numerical analysis. Whereas the pre-factor C depends on N_e . It is 15 for $N_e = 2$ and 16 for $N_e = 3$. This scaling relation matches very closely to the previous analysis done by Gendiar *et al.*²⁸ where they have shown by using bosonization techniques and additional approximations that persistent current decays algebraically with increasing system size and the exponent becomes exactly 1.33 at half filling when $U = 1$.

Finally, in Fig. 9 we show the dependence of current with ring size N in the half-filled band case setting the Coulomb interaction strength $U = 1$. Since we restrict ourselves in the half-filled limit and due to our computation limitation, we cannot consider larger rings as the dimension of the matrix increases rapidly. Here, the red dots and the green lines represent the similar meaning as described in Fig. 8. Two cases are analyzed depending on the disorder strength W , and, in both cases we find the identical scaling relation like above i.e., $I \propto N^{-\xi}$, though the exponent changes with W . For $W = 0$ we get $\xi = 1.5$, while it is 1.4 for $W = 2$. Most notably, from our exhaustive numerical analysis we find that with

increasing disorder strength ξ gradually decreases and eventually reach towards the limiting value 1.33, which is consistent with the asymptotic behavior as suggested by Gendiar *et al.*²⁸.

IV. SUMMARY

To summarize, in the present work we have studied persistent current in a 1D mesoscopic ring of spinless fermions with nearest-neighbor Coulomb interaction. Considering the interacting Hamiltonian *exactly* we have determined the energy eigenvalues through exact numerical diagonalization and computed persistent current using conventional derivative method. In addition we have also discussed conducting properties of the system by calculating Drude weight as a function of Coulomb correlation. From our analysis we have clearly shown that with increasing Coulomb correlation half-filled rings exhibit a metal-to-insulator transition, while, for less than half-filling only metallic phase is obtained irrespective of the strength of U . At the end, we have discussed scaling behavior of persistent current to address its asymptotic nature with ring size N .

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